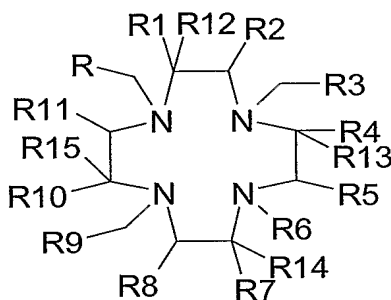


We claim:

1. A compound comprising a polyazamacrocyclic compound and at least one phosphonic group substituted on at least one of the aza groups of said polyazamacrocyclic compound.

2. The compound of claim 1 wherein said polyazamacrocyclic compound comprises the general formula (II):



(II)

where $R^1 = R^2 = R^7 = R^8 = R^{10} = R^{11} = H$;

$R^{12}, R^{13}, R^{14}, \text{ and } R^{15} = CH_3 \text{ or } H$;

$R^4 = R^5$; and $R^{10} = R^{11}$ can be H or groups taken together forming a cyclic C_3 - C_4 alkene group;

at least one of R, R^3 , R^6 or $R^9 = X$, where $X = CH_2P(O)(OH)_2$, CH_2P

$(O)(OC_4H_9-t)_2$, $CH_3CHP(O)(OH)_2$, $CHP(O)(OH)_2-$

$(CH_2)_nCO_2H$, $CHP(O)(OH)_2$, $(CH_2)_nNH_2$, $CHP(O)(OH)_2-$

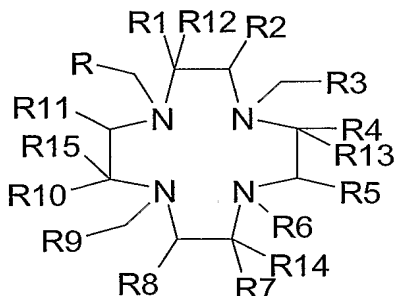
Aryl- CO_2H , $CHP(O)(OH)_2$ -Aryl- NH_2 or $CHP(O)(OH)_2-$

Aryl- $NHCS$, where $n = 1-12$; and

when R, R^3 , R^6 or R^9 are not X, then that R, R^3 , R^6 or R^9 is CO_2C

$(CH)_3$, or CO_2H .

3. The compound of claim 1 wherein said polyazamacrocyclic compound comprises the general formula (III):



(III)

where $R = R^3 = R^9 = \text{CO}_2\text{C}(\text{CH}_3)_3$, or CO_2H ;

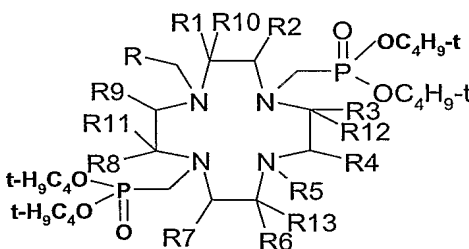
$R^1 = R^2 = R^4 = R^5 = R^7 = R^8 = R^{10} = R^{11} = \text{H}$;

R^{12}, R^{13}, R^{14} , and $R^{15} = \text{CH}_3$ or H ;

$R^{10} = R^{11}$ can be H or groups taken together forming a cyclic $\text{C}_3\text{-C}_4$ alkene group; and

$R^6 = \text{CH}_2\text{P}(\text{O})(\text{OH})_2$, $\text{CH}_2\text{P}(\text{O})(\text{OC}_4\text{H}_9\text{-t})_2$, $\text{CH}_3\text{CHP}(\text{O})(\text{OH})_2$, $\text{CHP}(\text{O})(\text{OH})_2\text{-(CH}_2)_n\text{CO}_2\text{H}$, $\text{CHP}(\text{O})(\text{OH})_2\text{, (CH}_2)_n\text{NH}_2$, $\text{CHP}(\text{O})(\text{OH})_2\text{-Aryl-CO}_2\text{H}$ or $\text{CHP}(\text{O})(\text{OH})_2\text{-Aryl-NH}_2$, where $n = 1\text{-}12$.

4. The compound of claim 1 wherein said polyazamacrocyclic compound comprises the general formula (IV):



(IV)

where $R^1 = R^2 = R^3 = R^4 = R^6 = R^7 = R^8 = R^9 = \text{H}$;

$R^3 = R^4$ and $R^8 = R^9$ can be H or groups taken together forming a cyclic C₃-C₄ alkene group;

R^{10} , R^{11} , R^{12} and $R^{13} = CH_3$ or H;

$R = CO_2C(CH_3)_3$; and

$R^5 = CH_2P(O)(OH)_2$, $CH_2P(O)(OC_4H_9-t)_2$, $CH_3CHP(O)(OH)_2$,

$CHP(O)(OH)_2-(CH_2)_nCO_2H$, $CHP(O)(OH)_2$, $(CH_2)_nNH_2$,

$CHP(O)(OH)_2-Aryl-CO_2H$, $CHP(O)(OH)_2-Aryl-NH_2$ or CH

$P(O)(OH)_2-Aryl-NHCS$, where n = 1-12.

5. A compound of the formula:

10-Phosphonomethyl-1,4,7,10-tetraazacyclododecane-1,4,7-triacetic acid (MPDO3A);

10-(1-phosphonoethyl)-1,4,7,10-tetraazacyclododecane-1,4,7-triacetic acid;

10-[[Bis(1,1-dimethylethoxy)phosphinyl]methyl]-1,4,7,10-

tetraazacyclododecane-1,4,7-triacetic acid 1,7-bis(1,1-dimethylethyl)ester;

10-[[Bis(1,1-dimethylethoxy)phosphinyl]methyl]- α' -(carboxymethyl)-

1,4,7,10-tetraazacyclododecane-1,4,7-triacetic acid $\alpha, \alpha', \alpha''$ -tris(1,1-dimethylethyl)ester;

10-[[1-[Bis(1,1-dimethylethoxy)phosphinyl]-3-carboxy]propyl]-

1,4,7,10-tetraazacyclododecane-1,4,7-triacetic $\alpha, \alpha', \alpha''$ -tris(1,1-dimethylethyl)ester; or

4,10-Bis[[bis(1,1-dimethylethoxy)phosphinyl]methyl]-1,4,7,10-

tetraazacyclododecane-1,7-diacetic (1,1-dimethylethyl)ester.

6. A compound comprising a homo dimer, hetero dimer, homo multimer or hetero multimer of the compound of any of claims 1-5.

7. A complex comprising the compound of any of claims 1-5 complexed with a paramagnetic or radionuclide metal.

8. A method for preparing a complex comprising the step of conjugating the compound of any of claims 1-5 with a paramagnetic or radionuclide metal.

5 9. A method of imaging comprising the steps of:
administering to a patient a diagnostic imaging agent comprising the compound of any of claims 1-5 complexed with a paramagnetic or radionuclide metal, and
imaging said patient.

10 10. A method for preparing a diagnostic imaging agent comprising the step of
adding to an injectable medium a substance comprising the compound of any of claims 1-5.

11. A kit for preparing a diagnostic imaging agent comprising the compound of any of claims 1-5.

12. A kit for preparing a radiotherapeutic agent comprising the compound of any of claims 1-5.

15 13. A method of treating a patient comprising the step of administering to a patient a radiotherapeutic agent comprising the compound of any of claims 1-5 complexed with a therapeutic radionuclide.

14. A method of preparing a radiotherapeutic agent comprising the step of adding to an injectable therapeutic medium a substance comprising at least one compound of any of
20 claims 1-5.

15. The compound of any of claims 1-5 further comprising a linking group.

16. The complex of claim 7 further comprising a linking group.

17. The compound of any of claims 1-5 further comprising a targeting moiety.

18. The complex of claim 7 further comprising a targeting moiety.

19. The compound of any of claims 1-5 further comprising a linking group and a targeting moiety.

20. The complex of claim 7 further comprising a linking group and a targeting moiety.

5 21. A salt form of the compound of any of claims 1-5.

22. A salt form of the complex of claim 7.

23. A method for preparing a polyazamacrocyclic compound bound to a linker, targeting moiety, diagnostic moiety or therapeutic moiety comprising the step of:

conjugating a polyazamacrocyclic compound to a linker, targeting moiety,

10 diagnostic moiety or therapeutic moiety with a coupling agent, wherein:

said coupling agent is selected from the group consisting of DCC, HOBT and HATU,

said polyazamacrocyclic compound comprises one carboxyl group and/or at least one amino group, and

15 said linker, targeting moiety, diagnostic moiety or therapeutic moiety comprises at least one amino or acid functional group.